



Safety,
Health,
Environmental,
and
Regulatory
Affairs

EDTN
HPV Robust Summaries
Akzo Nobel Functional Chemicals LLC
December 2002

20021226141800

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1. Substance Information

<i>CAS Number:</i>	5766-67-6
<i>Chemical Name:</i>	Acetonitrile, 2, 2', 2'', 2'''-(1,2-ethanediyldinitrilo) tetrakis-
<i>Structural Formula:</i>	C10H12N6
<i>Other Names:</i>	Acetonitrile, (ethylenedinitrilo) tetra-; EDTN
<i>Exposure Limits:</i>	None

2. Physical – Chemical Properties

2.1. Melting Point:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038
Method:	OECD 102
GLP:	Yes
Year:	1998
Value:	73-74°C
Decomposition:	At temperatures above 231°C
Conclusions:	The melting point of PDTN is 73-74°C.
Reliability:	1
Reference:	1
Remarks:	None
Additional	None
References for Melting Point Studies:	

Identity:	EDTN; CAS# 5766-67-6
Method:	EPIWIN Computer Model
GLP:	Not applicable
Year:	Not applicable
Value:	159°C
Decomposition:	Not available
Conclusions:	The melting point of EDTN is estimated to be 159°C.
Reliability:	1
Reference:	2
Remarks:	None

Additional
References for
Melting Point
Studies: None

2.2. Boiling Point:

Identity: EDTN; CAS# 5766-67-6
Method: EPIWIN Computer Model
GLP: Not applicable
Year: Not applicable
Value: 427.17°C
Decomposition: Not available
Conclusions: The boiling point of EDTN is estimated to be 427.17°C.
Reliability: 1
Reference: 3
Remarks: None
Additional
References for
Melting Point
Studies: None

2.3. Density:

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 109
GLP: Yes
Year: 1998
Value: 1.23 g/cm³
Conclusions: The density of PDTN is 1.23 g/cm³.
Reliability: 1
Reference: 4
Remarks: None
Additional
References for
Density Studies: None

2.4. Vapor Pressure:

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 104
GLP: Yes

Year: 1998
Value: 0.19 ± 2 Pa = $1.43 \pm 0.15 \times 10^{-3}$ mmHg
Temperature° C: 20
Pressure Unit: Pa or mmHg
Decomposition: No
Conclusions: The vapor pressure of PDTN at 20°C is 0.19 ± 2 Pa = $1.43 \pm 0.15 \times 10^{-3}$ mmHg.
Reliability: 1
Reference: 5
Remarks: Static technique was used in the study
Additional: None
Reference for Vapor Pressure Studies:

Identity: EDTN; CAS# 5766-67-6
Method: EPIWIN Computer Model
GLP: Not applicable
Year: Not applicable
Value: 7.54×10^{-8} mmHg
Temperature° C: 25
Pressure Unit: mm Hg
Decomposition: Not available
Conclusions: The vapor pressure of EDTN at 25°C is estimated to be 7.54×10^{-8} mmHg.
Reliability: 1
Reference: 6
Remarks: None
Additional: None
Reference for Vapor Pressure Studies:

2.5. Partition Coefficient (log Kow):

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: 107
GLP: Yes
Year: 1998
Log Kow: -1.3

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Temperature°C: 40
Conclusions: The log Kow of PDTN is -1.3.
Reliability: 1
Reference: 7
Remarks: None
Additional: None
References for
Partition
Coefficient Studies:

Identity: EDTN; CAS# 5766-67-6
Method: EPIWIN Computer Model
GLP: Not applicable
Year: Not applicable
Log Kow: -2.17
Temperature°C: Not available
Conclusions: The log Kow of EDTN is estimated to be -2.17.
Reliability: 1
Reference: 8
Remarks: None
Additional: None
References for
Partition
Coefficient Studies:

2.6. Water Solubility:

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: 105
GLP: Yes
Year: 1998
Value at
temperature°C: 1.67g/L at 18±1.5°C
Description of
solubility: Clear
PH value and
concentration at
temperature °C: 7.8-8.1 at 18±1.5°C

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Pka value at 25°C: Not reported
Conclusions: The water solubility of PDTN is 1.67 g/L.
Reliability: 1
Reference: 9
Remarks: None
Additional: None
References for Water Solubility Studies:

Identity: EDTN; CAS# 576-67-6
Method: EPIWIN Computer Model
GLP: Not applicable
Year: Not applicable
Value at 1000 g/L at 25°C
temperature°C:
Description of solubility: Not available
PH value and concentration at temperature °C: Not available
Pka value at 25°C: Not available
Conclusions: The water solubility of EDTN is estimated to be 1000 g/L.
Reliability: 1
Reference: 10
Remarks: None
Additional: None
References for Water Solubility Studies:

3. Environmental Fate

3.1. Photodegradation:

Identity: EDTN; CAS# 5766-67-6
Method: EPIWIN Computer Model
GLP: Not applicable
Type: Not applicable
Year: Not applicable

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Light Source: Not applicable
 Light Spectrum (nm): Not applicable
 Half-life: 4.589 hours
 Breakdown Products: Not available
 Conclusions: The half-life in the atmosphere for EDTN is estimated to be 4.589 hours.
 Reference: ¹¹
 Remarks: None
 Additional: None
 References for Photodegradation Studies:

3.2. Stability in Water:

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
 Method: EEC Directive 92/69, Part C Publication L383 1992
 GLP: Yes
 Type: Hydrolysis as a function of pH
 Year: 1999
 Half-life at a specific pH:
 pH 4: 5.3 years at 25°C
 pH 7: 3.9 years at 25°C
 pH 9: 0.3 years at 25°C
 Breakdown Products: Not determined
 Conclusions: The half-life of PDTN at pH 4, 7 and 9 at 25°C is 5.3, 3.9 and 0.3 years, respectively.
 Reliability: ¹
 Reference: ¹²
 Remarks: Half-life at 25°C estimated from data of studies at higher temperatures.
 Additional References for Stability in Water Studies: None

3.3. Transport (Fugacity):

Identity: EDTN; CAS# 5766-67-6
 Method: EPIWIN Computer Model
 GLP: Not applicable
 Type: Not applicable
 Year: Not applicable
 Media: Air, Water, Soil, Sediment

Distributions:	Compartment	Released 100% to air	Release 100% to water	Release 100% to soil
	Air	3.99 x 10 ⁻¹⁴	3.3 x 10 ⁻³¹	7.07 x 10 ⁻²⁹
	Water	39.8	99.8	36
	Soil	60.2	4.98 x 10 ⁻¹⁶	64
	Sediment	0.0753	0.189	0.0681
Conclusions:	EDTN is distributed primarily to water and soil.			
Reliability:	1			
Reference:	13			
Remarks:	When released equally to air, water and soil, EDTN is distributed 51.8% to water and 48.1% to soil.			
Additional References for Transport (Fugacity) Studies:	None			

3.4. Biodegradation:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038
Method:	OECD 301
Type:	Modified Sturm Test
GLP:	Yes
Year:	1998
Degradation% after time:	0% at 28 days
Breakdown	Not determined
Products:	
Concentration Of Test Chemical:	12 mg TOC/L
pH Of Test Media:	7.8-8.1
Conclusions:	PDTN is not readily biodegradable.
Reliability:	1
Reference:	14
Remarks:	Source of test organism was activated sludge obtained from a municipal sewage treatment plant
Additional References for Biodegradation Studies:	None

4. Ecotoxicity

4.1. Acute Toxicity to Fish:

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038

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Method: 203
 Type: Static
 GLP: Yes
 Year: 1998
 Species/Strain: Zebra fish/Teleostie, Cyprinidae
 Supplier: Charles River Aquatics, The Netherlands
 Analytical: Gas Chromatography
 Monitoring:
 Exposure Period: 96 hours
 Nominal/Measured Concentrations: 100 mg/L; 107-109 mg/L
 LC50: >100 mg/L
 Conclusions: The LC50 of PDTN in zebra fish is >100 mg/L.
 Reliability: 1
 Reference: 15
 Remarks: There was no mortality during the study. Ten fish were used in the test group. The water hardness was 250 mg/CaCO3/L. The pH was 7.2-8.2. The temperature was 20.7-21.3°C. The DO was 4.7-9.
 Additional References for Acute Toxicity to Fish Studies: None

4.2. Acute Toxicity to Invertebrates:.

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
 Method: 202
 Type: Static
 GLP: Yes
 Year: 1998
 Species/Strain: Daphnia magna/Crustacea, Cladocera Strauss, 1820
 Supplier: Not available
 Analytical: Gas Chromatography
 Monitoring:
 Exposure Period: 48 hours
 Nominal/Measured Concentrations: 1, 10, 100 mg/L; 110 mg/L
 EC50: >100 mg/L
 Conclusions: The EC50 of PDTN in Daphnia magna is >100 mg/L.
 Reliability: 1
 Reference: 16

Remarks: There was no mortality during the study. Ten fish were used at 1 and 10 mg/L and 20 fish in the 100 mg/L group. The water hardness was 250 mg/CaCO₃/L. The pH was 8.0-8.3. The temperature was 21.0-21.3°C. The DO was 8.8-8.9.

Additional References for Acute Toxicity to Invertebrates Studies: None

4.3. Acute Toxicity to Aquatic Plants:

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: 201
Type: Growth Inhibition Test
GLP: Yes
Year: 1998
Species/Strain/Supplier: Selenastrum capricornutum/CCAP 278/4/Not available
Analytical Monitoring: Gas Chromatography
Exposure Period: 72 hours
Nominal/Measured Concentrations: 10, 18, 32, 56, 100 and 180 mg/L/10.5, 34, 189
EC50: Growth inhibition – 60 mg/L; Growth rate reduction – 129 mg/L
Conclusions: The EC50 in algae for growth inhibition and growth rate reduction for PDTN is 60 and 129 mg/L, respectively.
Reliability: 1
Reference: 17
Remarks: Three replicates of the test concentrations were done. The water hardness was Ca+Mg: 0.24 mmol/L (24 mg CaCO₃/L). The pH was 8.1-8.4. The temperature was 21.2-23.0°C. The DO was 8.8-8.9.

Additional References for Acute Toxicity to Aquatic Plants Studies: None

5. Mammalian Toxicity

5.1. Acute Toxicity:

5.1.1. Oral

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 423
Type: Acute Toxic Class Method
GLP: Yes
Year: 1998
Species/Strain: Rat/Wistar Cr1(WI)
Sex: M/F
No. Of Animals Per 3
Sex Per Dose:
Vehicle: Polyethylene glycol
Route Of Administration: Oral gavage
Time Of Observation Period: 15 Days
Doses Administered: 2000 mg/kg
LD50: >2000 mg/kg
Conclusions: The oral LD50 of PDTN in rats is greater than 2000 mg/kg.
Reliability: 1
Reference: 18
Remarks: One female was found dead on day 3. Clinical signs of toxicity were lethargy, hunched posture, piloerection, diarrhea and red staining of the snout between days 1 and 3. Macroscopic examination showed hemorrhagic content of the urinary bladder in the animal that died. There were no effects in surviving animals.
Additional References for Acute Oral Toxicity Studies: None

5.1.2. Dermal

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 402
Type: Acute Dermal
GLP: Yes
Year: 1998
Species/Strain: Rat/Wistar Cr1(WI)

Sex:	M/F
No. Of Animals Per	5
Sex Per Dose:	
Vehicle:	Polyethylene glycol
Route Of	Dermal
Administration:	
Time Of	15 Days
Observation	
Period:	
Doses	2000 mg/kg for 24 hours
Administered:	
LD50:	>2000 mg/kg
Conclusions:	The dermal LD50 of PDTN in rats is greater than 2000 mg/kg.
Reliability:	1
Reference:	19
Remarks:	There was no mortality. Clinical signs of toxicity were red staining of the neck in one female between days 3 and 7 and scabs or scales in the treated area of two other females between days 3 and 6. Macroscopic examination showed no abnormalities.
Additional	None
References for	
Acute Dermal	
Toxicity Studies:	

5.1.3. Skin Irritation

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038
Method:	OECD 404
Type:	Semi-Occlusive
GLP:	Yes
Year:	1998
Species/Strain:	Rabbit/New Zealand white
Sex:	M
No. Of Animals:	3
Vehicle:	Water
Route Of	Dermal
Administration:	
Time Of Exposure:	4 hours
Time Of	1, 24, 48 and 72 hours
Observation	
Period:	
Concentration Of	0.5g
Test Material:	
Results:	There was no erythema or edema at any observation period.

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Conclusions: PDTN was not irritating to rabbits following dermal exposure for 4 hours.
Reliability: 1
Reference: 20
Remarks: None
Additional: None
References for Acute Dermal Irritation Studies:

5.1.4. Sensitization

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 406
Type: Maximization Test
GLP: Yes
Year: 1998
Species/Strain: Guinea Pig/Dunkin Hartley
Sex: F
No. Of Animals: 10
Vehicle: Corn Oil
Route Of Administration: Dermal
Time Of Observation Period: 24 Days
Concentration Of Test Material: Induction: Day 1 – 0.1%; Day 8 – 50%; Challenge: Day 21 – 50%
Results: There was no irritation seen 24 or 48 hours after challenge application.
Conclusions: PDTN was not sensitizing to guinea pigs at a 50% challenge concentration.
Reliability: 1
Reference: 21
Remarks: Alpha-hexylcinnamic aldehyde was the positive control.
Additional: None
References for Acute Dermal Sensitization Studies:

5.2. Repeated Dose Toxicity:

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 407
Type: 28-Day Oral Toxicity

GLP:	Yes
Year:	1998
Species/Strain:	Rat/Wistar Cr1(WI)BR
Sex:	M/F
No. Of Animals Per	20
Sex Per Dose:	
Vehicle:	Polyethylene glycol
Route of Administration:	Oral gavage
Time of Observation Period:	28 Days
Doses Administered:	50, 200, 1000 mg/kg/day
Frequency of Treatment:	Once daily for 28 days, 7 days per week
NOAEL (NOEL):	200 mg/kg
LOAEL (LOEL):	1000 mg/kg
Toxic Response By Dose Level:	1000 mg/kg: Mortality – one female on day 23; Clinical signs – piloerection, hunched posture, severe brown staining of the fur, red discoloration of the urine of females; Clinical chemistry – Significant increase in alanine aminotransferase activity of males and females; Macroscopic exam - enlarged kidney and urinary bladder in female that died during the study; Organ weights – a minor significant increase in liver to body weight ration in males at 1000 mg/kg/day; Microscopic exam – minimal to slight centrilobular hepatocellular hypertrophy in males and females at 1000 mg/kg/day, female that died during the study had marked hydronephrosis, moderate tubular dilation and pyelonephritis and moderate inflammation of the urinary bladder. 200 mg/kg/day: Clinical signs – severe brown staining of the fur. 50 mg/kg/day: None
Conclusions:	PDTN administered daily by oral gavage to rats for 28 days resulted in signs of liver toxicity at 1000 mg/kg/day. The effects on the liver included an increased liver weight and alanine aminotransferase activity and microscopic changes. The NOAEL was 200 mg/kg/day.
Reliability:	1
Reference:	22
Remarks:	None
Additional References for Repeated Dose Toxicity Studies:	None

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5.3. Genetic Toxicity:

5.3.1. *In Vitro* Gene Mutations

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 471/472
Type: Ames Test
GLP: Yes
Year: 1998
Cell Type: Salmonella typhimurium TA1535, TA1537, TA98, TA100;
E.coli WP2uvrA
Metabolic Activation: Rat S9 induced by Aroclor 1254
Concentrations Tested: Without S9: 3, 10, 33, 100, 333, 1000, 3330, 5000
With S9: 100, 333, 1000, 3330, 5000
Vehicle: Dimethyl sulfoxide
Cytotoxic Concentration: No toxicity at any concentration.
Genotoxic Effects With Metabolic Activation: None
Genotoxic Effects Without Metabolic Activation: None
Conclusions: PDTN was not mutagenic in Salmonella typhimurium strains TA1535, TA1537, TA98, TA100 or E.coli strain WP2uvrA in the presence or absence of metabolic activation.
Reliability: 1
Reference: 23
Remarks: The test concentrations were tested in triplicate.
Additional References for *In Vitro* Gene Mutation Studies: None

5.3.2. *In Vitro* Chromosome Aberrations

Identity: PDTN; CAS# 110057-45-9; Batch JNN98038
Method: OECD 473
Type: In Vitro
GLP: Yes
Year: 1998
Cell Type: Cultured peripheral human lymphocytes
Metabolic Activation: Rat S9 induced by Aroclor 1254
Concentrations Tested: Without S9: 333, 1000, 3330 (24 and 48 hour treatment)

Tested: With S9: 100, 333, 1000, 3330, 5000 (3 hour treatment)
Vehicle: Dimethylsulfoxide
Cytotoxic Concentration: No toxicity at any concentration.
Genotoxic Effects With Metabolic Activation: None
Genotoxic Effects Without Metabolic Activation: None
Conclusions: PDTN was not clastogenic in cultured peripheral human lymphocytes in the presence and absence of metabolic activation.
Reliability: 1
Reference: 24
Remarks: The test concentrations were tested in duplicate.
Additional References for *In Vitro* Chromosome Aberration Studies: None

References

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- 1 Determination Of The Melting Temperature Of PDTN. NOTOX Project No. 234822
11/19/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 2 EPIWIN 3.10 U.S. Environmental Protection Agency 2000
 - 3 EPIWIN 3.10 U.S. Environmental Protection Agency 2000
 - 4 Determination Of The Density Of PDTN. NOTOX Project No. 234844
10/21/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 5 Determination Of The Vapour Pressure Of PDTN. NOTOX Project No. 234855
10/21/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 6 EPIWIN 3.10 U.S. Environmental Protection Agency 2000
 - 7 Determination Of The Partition Coefficient (N-Octanol/Water) Of PDTN.
NOTOX Project No. 234855 10/21/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 8 EPIWIN 3.10 U.S. Environmental Protection Agency 2000
 - 9 Determination Of The Water Solubility Of PDTN.
NOTOX Project No. 234877 11/2/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 10 EPIWIN 3.10 U.S. Environmental Protection Agency 2000
 - 11 EPIWIN 3.10 U.S. Environmental Protection Agency 2000
 - 12 Determination Of The Hydrolysis Of PDTN As A Function Of pH.
NOTOX Project No. 258582 4/9/99. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 13 EPIWIN 3.10 U.S. Environmental Protection Agency 2000
 - 14 Determination Of 'Ready' Biodegradability: Carbon Dioxide (CO₂) Evolution Test
(Modified Sturm Test) With PDTN. NOTOX Project No. 235057 9/11/98.
Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 15 96-Hour Acute Toxicity Study In Zebra-Fish With PDTN (Static).
NOTOX Project No. 235068 10/29/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 16 Acute Toxicity Study In Daphnia Magna With PDTN (Static).
NOTOX Project No. 235079 10/29/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
 - 17 Fresh Water Algal Growth Inhibition Test With PDTN.
NOTOX Project No. 235081 10/29/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

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- 18 Assessment Of Acute Oral Toxicity With PDTN In The Rat (Acute Toxic Class Method).
NOTOX Project No. 234967 9/23/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
- 19 Assessment Of Acute Dermal Toxicity With PDTN In The Rat.
NOTOX Project No. 234978 9/23/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
- 20 Primary Skin Irritation/Corrosion Study With PDTN In The Rabbit
(4-Hour Semi-Occlusive Application). NOTOX Project No. 234989 9/23/98.
Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
- 21 Assessment Of Contact Hypersensitivity To PDTN In The Albino Guinea Pig (Maximization-Test).
NOTOX Project No. 235002 10/26/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
- 22 Subacute 28-Day Oral Toxicity With PDTN By Oral Gavage In The Rat.
NOTOX Project No. 235024 11/19/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
- 23 Evaluation Of The Mutagenic Activity Of PDTN In The Salmonella Typhimurium Reverse
Mutation Assay And the Escherichia Coli Reverse Mutation Assay (With Independent Repeat).
NOTOX Project No. 235035 9/7/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands
- 24 Evaluation Of The Ability Of PDTN To Induce Chromosome Aberrations In Cultured
Peripheral Human Lymphocytes. NOTOX Project No. 235046 10/30/98.
Sponsor: Akzo Nobel Chemicals B.V. The Netherlands